

PROPERTY OF
ANL-W Technical Library

Argonne National Laboratory

HARTREE-FOCK
SELF-CONSISTENT FIELD CALCULATIONS
FOR IRIDIUM

by

L. W. Panek and G. J. Perlow

The facilities of Argonne National Laboratory are owned by the United States Government. Under the terms of a contract (W-31-109-Eng-38) between the U. S. Atomic Energy Commission, Argonne Universities Association and The University of Chicago, the University employs the staff and operates the Laboratory in accordance with policies and programs formulated, approved and reviewed by the Association.

MEMBERS OF ARGONNE UNIVERSITIES ASSOCIATION

The University of Arizona	Kansas State University	The Ohio State University
Carnegie-Mellon University	The University of Kansas	Ohio University
Case Western Reserve University	Loyola University	The Pennsylvania State University
The University of Chicago	Marquette University	Purdue University
University of Cincinnati	Michigan State University	Saint Louis University
Illinois Institute of Technology	The University of Michigan	Southern Illinois University
University of Illinois	University of Minnesota	University of Texas
Indiana University	University of Missouri	Washington University
Iowa State University	Northwestern University	Wayne State University
The University of Iowa	University of Notre Dame	The University of Wisconsin

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

Printed in the United States of America

Available from

Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151
Price: Printed Copy \$3.00; Microfiche \$0.65

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

HARTREE-FOCK
SELF-CONSISTENT FIELD CALCULATIONS
FOR IRIDIUM

by

L. W. Panek and G. J. Perlow

Physics Division

November 1969

TABLE OF CONTENTS

	Page
ABSTRACT	v
I. INTRODUCTION	1
II. TABLES OF ATOMIC PARAMETERS	3
III. ENERGY LEVELS	33
IV. CALCULATIONS OF ELECTRON DENSITIES	36
V. ANALYTICAL FIT TO DENSITY CALCULATIONS	38
ACKNOWLEDGMENTS	42

LIST OF TABLES

Table I. HFSCF parameters for various outer-electron configurations
of iridium.

Table II. Electron densities for various outer-electron configurations
of iridium.

LIST OF FIGURES

Fig. 1. One-electron energies $\epsilon_{n\ell, n\ell}$ vs outer electron configuration
for the neutral atom Ir⁰.

Fig. 2. One-electron energies $\epsilon_{n\ell, n\ell}$ vs ionization state for the
5d^N 6s6p configuration.

Fig. 3. HFSCF electron-density calculations and the analytical fit
to Eq. (6).

ABSTRACT

Nonrelativistic Hartree-Fock self-consistent field (HFSCF) calculations have been carried out for a set of 55 outer-electron configurations (core) $5d^N 6s^M 6p^K$ in iridium ($Z=77$) by use of the CDC-3600 computer and the program of Froese and Wilson. Of central interest are the calculation of the electron density at the nucleus, $\rho(0)$, as a function of N , M , and K and a fit by an analytical expression containing lowest order shielding effects. The calculations are a basis for a quantitative study of the isomer shifts in the Mössbauer spectra of iridium compounds. In addition to $\rho(0)$, we report the values of the one-electron energy parameters, the mean values of various functions of r , the screening parameters, and the initial slope parameter a_{nl} .

I. INTRODUCTION

This report presents results obtained with the restricted nonrelativistic Hartree-Fock self-consistent field (HFSCF) program of C. Froese and M. Wilson.¹ The program is designed for use on the CDC-3600 computer.

The main purpose of these calculations was to obtain the total electron density at the nucleus for various outer-electron configurations of iridium. Fifty-five such configurations were studied. The aim is to form a basis for an understanding of the isomer shifts in the Mössbauer spectra of iridium compounds in terms of the populations in the valence shells. To organize the considerable amount of computer output, we have presented it both in graphical form (Fig. 3) and in the form of analytical expressions [Eqs. (6) and (6')] which we regard as the most useful result of the study.

The computer output contains a great deal of additional information—some of which (e.g., values of $\langle 1/r^3 \rangle$) is relevant to the Mössbauer effect but most of which is not. Since the effort involved in tabulating the other results is small, we have supplied most of them but have stopped short of actually listing the wave functions.

In general the HFSCF description assumes that the total wave function for a many-electron system is a linear combination of Slater determinants composed of single-electron wave functions whose orbital parts are of the form

$$\Psi_{n,\ell} = R_{n,\ell}(r) Y_{\ell}^m(\theta, \phi). \quad (1)$$

The normalization is,

$$\int R_{n,\ell}^*(r) R_{n',\ell'}(r) r^2 dr = \delta_{nn'} \delta_{\ell\ell'} \quad (2)$$

and

¹C. Froese Fisher and M. Wilson, Programs for Atomic-Structure Calculations (Argonne National Laboratory, Argonne, Illinois, 1968), Report No. ANL-7404.

$$\int Y_l^{m^*}(\theta, \varphi) Y_{l'}^{m'}(\theta, \varphi) d\Omega = \delta_{ll'} \delta_{mm'}. \quad (3)$$

In the nonrelativistic case, only the $\Psi_{n,0}(r)$ are nonzero at the origin, the total density being

$$\sum_n v_{n,0} |\Psi_{n,l}(0)|^2 = (1/4\pi) \sum_n v_{n,0} |R_{n,0}(0)|^2, \quad (4)$$

where $v_{n,l}$ is the population of the state n,l . We define

$$\rho(0) = \sum_n \rho_n(0) = \sum_n v_{n,0} |R_{n,0}(0)|^2. \quad (5)$$

The quantities $\rho_n(0)$ and $\rho(0)$ are tabulated for each configuration studied.

The iridium atom is sufficiently heavy that relativistic corrections to $\rho(0)$ are important. The theoretical work of Racah,² Rosenthal and Breit,³ and Bodmer⁴ in addition to a small number of relativistic HFSCF calculations⁵ has shown that the main effect of relativity is to multiply each $\rho_n(0)$ by a constant S' whose value to fair approximation is independent of n . For iridium Shirley⁶ calculates $S' = 6.2$. Thus while the relativistic effect is large, to this approximation it changes only the ordinate scale in Fig. 3 and the value of the multiplier A in Eq. (6'). Lacking relativistic calculations, we are forced to adopt an optimistic point of view concerning the merit of the approximation.

The Froese-Wilson program either calculates wave functions and atomic parameters for a selected term of the desired configuration (or in fact a mixture of configurations) or takes a suitable average (Av) over the configuration. To compare the two alternatives,

² G. Racah, Nature 129, 723 (1932).

³ J. E. Rosenthal and G. Breit, Phys. Rev. 41, 459 (1932); G. Breit, Rev. Mod. Phys. 30, 507 (1958).

⁴ A. R. Bodmer, Proc. Phys. Soc. (London) A66, 1041 (1953).

⁵ D. W. Hafemeister, J. Chem. Phys. 46, 1929 (1967).

⁶ D. A. Shirley, Rev. Mod. Phys. 36, 339 (1964).

the value of $\rho(0)$ for $5d^5 6s^2$ (Av) was compared with $5d^5 6s^2$ ⁶ (S), the Hund's rule ground state. The difference in $\rho(0)$ was hardly appreciable for the two cases. Accordingly, we have used the average over the configuration exclusively in the results we present.

Section II consists of a short explanation of each of the Hartree-Fock parameters and an extensive tabulation of them for iridium. Section III presents several one-electron energy-level diagrams. A discussion of the electron-density calculations follows in Section IV where the results are presented in tabular form. Finally (Section V) the calculated densities are fitted to a mathematical expression and the parameters are tabulated.

II. HARTREE-FOCK PARAMETERS FOR IRIDIUM

The results of the Hartree-Fock calculations for iridium are reported in the form of atomic parameters in Table I. The parameters listed are the following.

- (a) The one-electron diagonal energy parameters $\epsilon_{n\ell, n\ell}$ as defined by Hartree.⁷ The units are Rydbergs ($1\text{Ry} = 13.605 \text{ eV}$).
- (b) The values of $a_{n\ell} = R_{n\ell}(r)/r^\ell$ as $r \rightarrow 0$. Here r is given in units of the Bohr radius $a_0 = 0.52917 \text{ \AA}$. For s states, $a_{n,0}^2 = \rho_n(0)$.
- (c) The Hartree screening parameters defined as $\sigma_{n\ell} = Z - [\langle r \rangle_H / \langle r \rangle]$, where $\langle r \rangle$ is the expectation value of r obtained from the calculated HF radial wave function, and $\langle r \rangle_H$ is the expectation value in the same $n\ell$ state, calculated with hydrogenic wave functions of an atom with atomic number Z .
- (d) The expectation value of r , $\langle n\ell | r | n\ell \rangle$ in units of a_0 .
- (e) The expectation value of r^2 .
- (f) The expectation value of $1/r^3$.
- (g) The expectation value of r^4 .

⁷ D. R. Hartree, Calculation of Atomic Structures (John Wiley and Sons, New York, 1957), p. 54.

(h) The total energy of the atom or ion in units of Rydbergs.

With each value of N, calculations were performed for seven different outer-electron configurations. The ionization state varied from Ir I (Ir^0) to Ir X (Ir^{+9}). The seven classes are 5d^N , $5\text{d}^N 6\text{s}$, $5\text{d}^N 6\text{s}^2$, $5\text{d}^N 6\text{s} 6\text{p}$, $5\text{d}^N 6\text{s}^2 6\text{p}$, $5\text{d}^N 6\text{s} 6\text{p}^2$, and $5\text{d}^N 6\text{s}^2 6\text{p}^2$, where N varies from zero to $(9 - M - K)$, M and K being the number of 6s and 6p electrons, respectively.

TABLE I. HFSCF parameters for various outer-electron configurations of iridium

Ir ⁰ 5d ⁹								
nl	$\epsilon_{nl, nl}$	a _{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5132.409	1341.615	0.725	0.019666	0.000517	0.0000	0.000001	
2S	861.8115	446.1243	4.607	0.082881	0.008053	0.0000	0.000109	
2P	826.3552	9519.730	5.723	0.070149	0.005960	16055.3407	0.000069	
3S	203.8710	210.8692	12.512	0.209343	0.049948	0.0000	0.003724	
3P	187.2189	4765.889	14.461	0.199875	0.046189	3489.3660	0.003323	
3D	156.5649	22022.77	17.037	0.175109	0.035821	615.9508	0.002245	
4S	44.40231	103.9615	25.131	0.462708	0.241053	0.0000	0.083622	
4P	37.19339	2326.123	27.895	0.468382	0.248843	806.4857	0.091393	
4D	24.04938	11100.01	33.266	0.480100	0.266097	125.2469	0.112424	
4F	6.473564	11784.00	42.221	0.517550	0.324493	26.0440	0.217636	
5S	6.539834	42.02279	42.848	1.098031	1.353772	0.0000	2.715504	
5P	4.178305	882.7415	46.727	1.205700	1.648760	115.5858	4.234917	
5D	0.620644	3005.394	57.691	1.786747	3.907230	9.0094	33.464448	
Total Energy = -16806.200 Ry								

Ir ⁺¹ 5d ⁸								
nl	$\epsilon_{nl, nl}$	a _{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5133.211	1341.614	0.725	0.019666	0.000517	0.0000	0.000001	
2S	862.6190	446.1244	4.607	0.082881	0.008053	0.0000	0.000109	
2P	827.1723	9519.718	5.724	0.070150	0.005960	16055.3498	0.000069	
3S	204.6794	210.8697	12.512	0.209342	0.049948	0.0000	0.003724	
3P	188.0276	4765.899	14.461	0.199874	0.046189	3489.3824	0.003323	
3D	157.3771	22022.59	17.037	0.175109	0.035822	615.9473	0.002245	
4S	45.21266	103.9621	25.132	0.462710	0.241055	0.0000	0.083624	
4P	38.00365	2326.118	27.895	0.468384	0.248846	806.4807	0.091394	
4D	24.85858	11099.05	33.270	0.480220	0.266144	125.2269	0.112462	
4F	7.283206	11784.67	42.215	0.517466	0.324292	26.0451	0.216755	
5S	7.341182	42.74375	42.748	1.094842	1.344572	0.0000	2.660835	
5P	4.964562	887.8011	46.540	1.198278	1.624756	116.9118	4.05219	
5D	1.398769	3163.613	56.293	1.666113	3.288745	9.9716	20.325651	
Total Energy = -16805.953 Ry								

Table I. (Continued)

Ir⁺² 5d⁷

<i>n</i> <i>l</i>	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5134.172	1341.614	0.725	0.019666	0.000517	0.0000	0.000001
2S	863.5823	446.1237	4.608	0.082882	0.008053	0.0000	0.000109
2P	828.1355	9519.714	5.724	0.070149	0.005960	16055.3142	0.000069
3S	205.6406	210.8709	12.512	0.209342	0.049948	0.0000	0.003724
3P	188.9887	4765.934	14.460	0.199873	0.046188	3489.4248	0.003323
3D	158.3379	22022.59	17.038	0.175110	0.035822	615.9458	0.002245
4S	46.17261	103.9649	25.131	0.462701	0.241048	0.0000	0.083618
4P	38.96333	2326.162	27.894	0.468373	0.248834	806.5064	0.091381
4D	25.81618	11098.37	33.272	0.480244	0.266169	125.2132	0.112467
4F	8.241100	11787.43	42.197	0.517201	0.323786	26.0548	0.215161
5S	8.274140	42.95209	42.591	1.089839	1.330689	0.0000	2.587713
5P	5.873961	895.5607	46.279	1.188131	1.593405	118.9559	3.845825
5D	2.287900	3316.997	55.171	1.580468	2.907806	10.9479	14.664922

Total Energy = -16805.308 Ry

Ir⁺³ 5d⁶

<i>n</i> <i>l</i>	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5135.255	1341.614	0.725	0.019666	0.000517	0.0000	0.000001
2S	864.6643	446.1251	4.607	0.082881	0.008053	0.0000	0.000109
2P	829.2176	9519.743	5.723	0.070149	0.005960	16055.3363	0.000069
3S	206.7168	210.8740	12.512	0.209340	0.049947	0.0000	0.003724
3P	190.0653	4766.022	14.459	0.199870	0.046187	3489.5444	0.003323
3D	159.4144	22022.83	17.037	0.175108	0.035821	615.9569	0.002245
4S	47.24681	103.9694	25.129	0.462685	0.241031	0.0000	0.083602
4P	40.03711	2326.250	27.892	0.468354	0.248811	806.5646	0.091355
4D	26.88722	11097.78	33.274	0.480258	0.266176	125.2013	0.112440
4F	9.312730	11793.07	42.167	0.516748	0.322967	26.0753	0.212914
5S	9.303585	43.23419	42.390	1.083508	1.313545	0.0000	2.502667
5P	6.873456	905.3591	45.972	1.176367	1.558274	121.5650	3.630000
5D	3.261718	3465.970	54.206	1.513586	2.637094	11.9373	11.458281

Total Energy = -16804.200 Ry

Table I. (Continued)

Table I. (Continued)

Total Energy = -16797.825 Ry

Table I. (Continued)

 $\text{Ir}^{+8} \quad 5d^1$

$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5142.008	1341.611	0.725	0.019666	0.000517	0.0000	0.000001
2S	871.4259	446.1390	4.605	0.082879	0.008052	0.0000	0.000109
2P	835.9827	9519.998	5.721	0.070147	0.005959	16056.2103	0.000069
3S	213.4011	210.9129	12.503	0.209313	0.049934	0.0000	0.003722
3P	196.7551	4767.039	14.449	0.199837	0.046171	3490.9725	0.003320
3D	166.1098	22026.52	17.031	0.175090	0.035814	616.1019	0.002244
4S	53.87444	104.0409	25.097	0.462400	0.240705	0.0000	0.083302
4P	46.65925	2327.905	27.854	0.467990	0.248373	807.6792	0.090896
4D	33.48328	11103.46	33.236	0.479851	0.265579	125.3143	0.11492
4F	15.90902	11873.01	41.830	0.511793	0.314826	26.3558	0.195107
5S	15.41787	45.40547	41.006	1.041831	1.207419	0.0000	2.044920
5P	12.77831	972.0041	44.135	1.110614	1.376773	140.0409	2.698013
5D	9.034025	4160.609	50.503	1.302057	1.905573	17.0793	5.328417

Total Energy = -16790.692 Ry

 $\text{Ir}^{+9} \quad 5d^0$

$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5143.582	1341.610	0.725	0.019666	0.000517	0.0000	0.000001
2S	873.0032	446.1439	4.605	0.082878	0.008052	0.0000	0.000109
2P	837.5617	9520.080	5.720	0.070146	0.005959	16056.4408	0.000069
3S	214.9516	210.9256	12.500	0.209303	0.049929	0.0000	0.003721
3P	198.3075	4767.369	14.445	0.199825	0.046166	3491.4228	0.003319
3D	167.6649	22027.95	17.028	0.175082	0.035810	616.1597	0.002243
4S	55.40206	104.0668	25.085	0.462291	0.240580	0.0000	0.083189
4P	48.18508	2328.537	27.839	0.467852	0.248208	808.1063	0.090729
4D	35.00158	11106.97	33.218	0.479652	0.265306	125.3864	0.111119
4F	17.42712	11899.83	41.729	0.510335	0.312552	26.4484	0.190768
5S	16.78718	45.94050	40.688	1.032706	1.185315	0.0000	1.960076
5P	14.09857	987.3294	43.746	1.097602	1.343153	144.4690	2.549972

Total Energy = -16786.170 Ry

Table I. (Continued)

Total Energy = -16806.183 Ry

Table I. (Continued)

Ir⁺² 5d⁶ 6s

<i>n</i> <i>l</i>	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5134.519	1341.613	0.725	0.019666	0.000517	0.0000	0.000001
2S	863.9418	446.1260	4.617	0.082881	0.008053	0.0000	0.000109
2P	828.4931	9519.705	5.723	0.070149	0.005960	16055.3405	0.000069
3S	205.9978	210.8776	12.511	0.209338	0.049946	0.0000	0.003724
3P	189.3445	4766.018	14.459	0.199870	0.046187	3489.5589	0.003323
3D	158.6970	22022.59	17.037	0.175108	0.035821	615.9522	0.002245
4S	46.5382	103.9787	25.126	0.462664	0.241007	0.0000	0.083585
4P	39.31796	2326.166	27.893	0.468367	0.248829	806.5055	0.091370
4D	26.16701	11096.96	33.276	0.480286	0.266209	125.1849	0.112467
4F	8.593182	11791.73	42.171	0.516816	0.323069	26.0706	0.213132
5S	8.599074	43.28032	42.379	1.083165	1.313150	0.0000	2.506624
5P	6.16830	903.9987	46.039	1.178899	1.566631	121.1995	3.692350
5D	2.56478	3424.883	54.520	1.534725	2.724956	11.6595	12.544325
6S	1.667926	14.89811	58.094	2.856221	9.108890	0.0000	120.939855

Total Energy = -16805.036 Ry

Ir⁺³ 5d⁵ 6s

<i>n</i> <i>l</i>	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5135.634	1341.613	0.725	0.019666	0.000517	0.0000	0.000001
2S	865.0549	446.1275	4.607	0.082881	0.008053	0.0000	0.000109
2P	829.6062	9519.732	5.723	0.070149	0.005960	16055.3450	0.000069
3S	207.1031	210.8818	12.510	0.209335	0.049945	0.0000	0.003724
3P	190.4500	4766.114	14.458	0.199867	0.046185	3489.6493	0.003322
3D	159.7984	22022.87	17.037	0.175107	0.035821	615.9603	0.002245
4S	47.63251	103.9874	25.123	0.462634	0.240974	0.0000	0.083556
4P	40.41821	2326.270	27.891	0.468348	0.248801	806.5437	0.091335
4D	27.26366	11096.57	33.276	0.480286	0.266196	125.1766	0.112410
4F	9.690073	11799.45	42.133	0.516249	0.322072	26.0981	0.210575
5S	9.643788	43.60940	42.158	1.076277	1.294933	0.0000	2.420768
5P	7.170546	914.6086	45.721	1.166919	1.531617	124.0513	3.486794
5D	3.554518	3567.097	53.647	1.477301	2.502085	12.6309	10.136860
6S	2.391751	16.70262	56.529	2.637911	7.730132	0.0000	84.631592

Total Energy = -16803.823 Ry

Table I. (Continued)

	Ir^{+4}	$5d^4 6s$	$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5136.836	1341.612	0.725	0.019666	0.000517		0.0000		0.000001	
2S	866.2626	446.1291	4.607	0.082881	0.008053		0.0000		0.000109	
2P	830.8138	9519.755	5.723	0.070149	0.005960		16055.4413		0.00069	
3S	208.3017	210.8888	12.508	0.209330	0.049942		0.0000		0.003723	
3P	191.6490	4766.270	14.457	0.199861	0.046183		3489.8976		0.003322	
3D	160.9976	22023.23	17.036	0.175105	0.035820		615.9780		0.002244	
4S	48.82561	103.9999	25.118	0.462586	0.240924		0.0000		0.083512	
4P	41.60978	2326.475	27.886	0.468298	0.248744		806.7133		0.091275	
4D	28.45075	11096.60	33.273	0.480251	0.266141		125.1759		0.112300	
4F	10.87769	11810.08	42.083	0.515507	0.320805		26.1361		0.207551	
5S	10.76183	43.98929	41.909	1.068663	1.275162		0.0000		2.331471	
5P	8.249539	926.5260	45.378	1.154269	1.495605		127.2939		3.288172	
5D	4.598569	3706.657	52.850	1.428596	2.324528		13.6201		8.480286	
6S	3.170764	18.31039	55.183	2.475096	6.786136		0.0000		64.003860	

Total Energy = -16802.038 Ry

	Ir^{+5}	$5d^3 6s$	$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5138.129	1341.612	0.725	0.019666	0.000517		0.0000		0.000001	
2S	667.5603	446.1322	4.606	0.082880	0.008053		0.0000		0.000109	
2P	632.1117	9519.798	5.722	0.070148	0.005960		16055.6343		0.00069	
3S	209.5861	210.8968	12.506	0.209323	0.049939		0.0000		0.003723	
3P	192.9339	4766.460	14.455	0.199855	0.046180		3490.1655		0.003322	
3D	162.2832	22023.84	17.035	0.175102	0.035819		616.0041		0.002244	
4S	50.10070	104.0145	25.111	0.462530	0.240861		0.0000		0.083455	
4P	42.88314	2326.735	27.880	0.468241	0.248673		806.8929		0.091197	
4D	29.71897	11097.17	33.268	0.480198	0.266053		125.1878		0.112142	
4F	12.14631	11824.69	42.020	0.514581	0.319265		26.1875		0.204107	
5S	11.94240	44.41357	41.640	1.060527	1.254404		0.0000		2.241448	
5P	9.387685	939.4789	45.019	1.141305	1.459572		130.8636		3.100367	
5D	5.711127	3843.628	52.113	1.386292	2.178155		14.6247		7.269082	
6S	3.998946	19.77792	53.980	2.345827	6.085943		0.0000		50.800794	

Total Energy = -16799.811 Ry

Table I. (Continued)

Ir ⁺⁶ 5d ² 6s		nℓ	ε _{nℓ, nℓ}	a _{nℓ}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5139.510	1341.611		0.725	0.019666	0.000517	0.0000	0.000001	
2S	568.9408	446.1345		4.606	0.082880	0.008053	0.0000	0.000109	
2P	633.4930	9519.850		5.722	0.070148	0.005959	16055.7377	0.000069	
3S	210.9483	210.9060		12.504	0.209317	0.049936	0.0000	0.003722	
3P	194.2969	4766.653		14.453	0.199850	0.046177	3490.4582	0.003321	
3D	163.6478	22024.76		17.033	0.175097	0.035817	616.0355	0.002244	
4S	51.44948	104.0315		25.104	0.462463	0.240784	0.0000	0.083385	
4P	44.23016	2327.087		27.872	0.468161	0.248576	807.1296	0.091095	
4D	31.05998	11098.57		33.259	0.480098	0.265909	125.2153	0.11920	
4F	13.48717	11842.54		41.946	0.513497	0.317499	26.2500	0.200355	
5S	13.17807	44.87528		41.354	1.052019	1.233062	0.0000	2.152426	
5P	10.57832	953.2515		44.649	1.128242	1.424068	134.7135	2.924751	
5D	6.877161	3978.265		51.423	1.348849	2.054317	15.6452	6.343637	
6S	4.872101	21.13848		52.882	2.239027	5.539302	0.0000	41.678580	
Total Energy = -16796.999 Ry									

Ir ⁺⁷ 5d ¹ 6s		nℓ	ε _{nℓ, nℓ}	a _{nℓ}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5140.961	1341.611		0.725	0.019666	0.000517	0.0000	0.000001	
2S	870.3950	446.1398		4.605	0.082879	0.008052	0.0000	0.000109	
2P	834.9478	9519.929		5.721	0.070147	0.005959	16056.0827	0.000069	
3S	212.3815	210.9178		12.502	0.209308	0.049932	0.0000	0.003722	
3P	195.7312	4766.969		14.449	0.199837	0.046171	3490.8710	0.003320	
3D	165.0836	22025.73		17.032	0.175093	0.035815	616.0793	0.002244	
4S	52.86652	104.0545		25.094	0.462378	0.240685	0.0000	0.083294	
4P	45.64497	2327.580		27.860	0.468052	0.248447	807.4575	0.090963	
4D	32.46802	11100.76		33.247	0.479964	0.265717	125.2608	0.11637	
4F	14.89527	11863.97		41.861	0.512255	0.315519	26.3243	0.196390	
5S	14.46348	45.36857		41.055	1.043262	1.211457	0.0000	2.065610	
5P	11.81647	967.6750		44.271	1.115210	1.389418	138.8025	2.761572	
5D	8.092173	4110.609		50.769	1.319248	1.947505	16.6796	5.613137	
6S	5.786690	22.41467		51.864	2.148300	5.096984	0.0000	35.030080	
Total Energy = -16793.588 Ry									

Table I. (Continued)

Ir ⁺⁸ 5d ₀ 6s		<i>n</i> <i>l</i>	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5142.496		1341.610		0.725	0.019666	0.000517	0.0000	0.000001
2S	871.9246		446.1445		4.605	0.082878	0.008052	0.0000	0.000109
2P	836.4789		9520.029		5.720	0.070146	0.005959	16056.3338	0.000069
3S	213.8836		210.9307		12.499	0.209299	0.049927	0.0000	0.003721
3P	197.2349		4767.291		14.446	0.199826	0.046166	3491.3116	0.003320
3D	166.5897		22027.17		17.029	0.175086	0.035812	616.1322	0.002243
4S	54.34730		104.0796		25.083	0.462273	0.240566	0.0000	0.083186
4P	47.12342		2328.135		27.847	0.467929	0.248298	807.8325	0.090810
4D	33.93906		11103.79		33.230	0.479782	0.265469	125.3207	0.111292
4F	16.36598		11889.20		41.765	0.510860	0.313335	26.4114	0.192133
5S	15.79436		45.88928		40.746	1.034376	1.189854	0.0000	1.981787
5P	13.09839		982.6170		43.888	1.102309	1.355815	143.1010	2.610429
6S	6.740425		23.62211		50.909	2.069653	4.729593	0.0000	29.990703

Total Energy = -16789.576 Ry

Ir ⁰ 5d ₇ 6s ₂		<i>n</i> <i>l</i>	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5132.981		1341.614		0.725	0.019666	0.000517	0.0000	0.000001
2S	862.3995		446.1257		4.607	0.082881	0.008053	0.0000	0.000109
2P	826.9507		9519.700		5.724	0.070149	0.005960	16055.3256	0.000069
3S	204.4592		210.8752		12.512	0.209340	0.049947	0.0000	0.003724
3P	187.8054		4765.963		14.460	0.199871	0.046187	3489.4699	0.003323
3D	157.1539		22022.44		17.038	0.175110	0.035822	615.9459	0.002245
4S	44.99435		103.9780		25.126	0.462660	0.241007	0.0000	0.083589
4P	37.78114		2326.088		27.895	0.468385	0.248850	806.4549	0.091393
4D	24.63243		11097.55		33.275	0.480269	0.266196	125.1967	0.112481
4F	7.058242		11787.13		42.197	0.517196	0.323759	26.0540	0.215086
5S	7.101935		43.06873		42.532	1.087981	1.326244	0.0000	2.571929
5P	4.688118		894.9268		46.341	1.190531	1.602391	118.7889	3.930898
6S	0.493179		11.29409		61.675	3.523675	14.291610	0.0000	341.883323
5D	1.112423		3254.632		55.761	1.624395	3.114752	10.5442	18.110554

Total Energy = -16806.062 Ry

Table I. (Continued)

Ir ⁺¹ 5d ⁶ 6s ²							
nℓ	ε _{nℓ, nℓ}	a _{nℓ}	σ	⟨r⟩	⟨r ² ⟩	⟨1/r ³ ⟩	⟨r ⁴ ⟩
1S	5133.877	1341.615	0.725	0.019666	0.000517	0.0000	0.000001
2S	863.2935	446.1269	4.607	0.082881	0.008053	0.0000	0.000109
2P	827.8442	9519.723	5.723	0.070149	0.005960	16055.3333	0.000069
3S	205.3487	210.8800	12.511	0.209337	0.049945	0.0000	0.003724
3P	186.6944	4766.021	14.460	0.199871	0.046187	3489.5685	0.003323
3D	158.0424	22022.64	17.037	0.175109	0.035822	615.9542	0.002245
4S	45.88388	103.9861	25.124	0.462639	0.240984	0.0000	0.083569
4P	38.66868	2326.098	27.895	0.468383	0.248844	806.4620	0.091381
4D	25.51705	11096.46	33.278	0.480306	0.266231	125.1739	0.112483
4F	7.943755	11791.11	42.1/4	0.516850	0.323118	26.0681	0.213235
5S	7.959190	43.34882	42.341	1.081976	1.310122	0.0000	2.493116
5P	5.514373	903.1585	46.085	1.180668	1.572728	120.9758	3.742195
6S	1.078928	13.64740	59.246	3.041654	10.424706	0.0000	165.613026
5D	1.921507	3391.724	54.798	1.553904	2.808411	11.4376	13.697724
Total Energy = -16805.583 Ry							
Ir ⁺² 5d ⁵ 6s ²							
nℓ	ε _{nℓ, nℓ}	a _{nℓ}	σ	⟨r⟩	⟨r ² ⟩	⟨1/r ³ ⟩	⟨r ⁴ ⟩
1S	5134.893	1341.613	0.725	0.019666	0.000517	0.0000	0.000001
2S	864.3214	446.1280	4.607	0.082881	0.008053	0.0000	0.000109
2P	828.8711	9519.712	5.723	0.070149	0.005960	16055.4000	0.000069
3S	206.3725	210.8849	12.510	0.209334	0.049944	0.0000	0.003723
3P	189.7177	4766.111	14.459	0.199868	0.046185	3489.7064	0.003322
3D	159.0655	22022.67	17.037	0.175109	0.035821	615.9579	0.002245
4S	46.90530	103.9973	25.119	0.462601	0.240944	0.0000	0.083537
4P	39.68793	2326.188	27.892	0.468360	0.248818	806.5210	0.091350
4D	26.53250	11095.82	33.278	0.480309	0.266226	125.1602	0.112438
4F	8.959568	11797.56	42.140	0.516345	0.322218	26.0918	0.210878
5S	8.930514	43.67880	42.121	1.075153	1.292136	0.0000	2.408781
5P	6.450407	913.0245	45.791	1.169519	1.539956	123.6237	3.545864
6S	1.745650	15.57532	57.460	2.763592	8.525891	0.0000	105.779051
5D	2.836582	3529.107	53.923	1.494985	2.572856	12.3672	10.943388
Total Energy = -16804.687 Ry							

Table I. (Continued)

Ir^{+3}	$5d^4 6s^2$	ϵ_{nl}	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5136.029	1341.613		0.725	0.019666	0.000517	0.00000	0.000001
2S	865.4604	446.1292		4.607	0.082881	0.008153	0.0000	0.000109
2P	830.0989	9519.729		5.723	0.070149	0.005960	16055.3750	0.000069
3S	207.5022	210.8921		12.508	0.209328	0.049941	0.0000	0.003723
3P	190.8474	47665.250		14.457	0.199862	0.046183	3489.8856	0.003322
3D	160.1952	22022.98		17.036	0.175106	0.035821	615.9633	0.002245
4S	48.03016	104.0085		25.116	0.462567	0.240903	0.0000	0.083499
4P	40.81054	2326.327		27.889	0.468327	0.248777	806.6168	0.091303
4D	27.65062	11095.48		33.277	0.480296	0.266195	125.1526	0.112353
4F	10.07827	11807.19		42.094	0.515674	0.321060	26.1259	0.208065
5S	9.987743	44.05732		41.876	1.067637	1.272661	0.0000	2.321153
5P	7.468440	924.2686		45.466	1.157481	1.505458	126.6763	3.351384
6S	2.476449	17.25598		55.985	2.569633	7.334571	0.0000	76.131163
5D	3.831431	3665.409		53.122	1.444865	2.385430	13.3236	9.077034

Total Energy = -16803.304 Ry

Ir^{+4}	$5d^3 6s^2$	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5137.254		1341.612	0.725	0.019666	0.000517	0.0000	0.000001
2S	866.6932		446.1324	4.606	0.082880	0.008053	0.0000	0.000109
2P	831.2422		9519.759	5.723	0.070149	0.005960	16055.5217	0.000069
3S	208.7235		210.8997	12.506	0.209322	0.049938	0.0000	0.003723
3P	192.0688		4766.407	14.455	0.199856	0.046180	3490.1026	0.003322
3D	161.4170		22023.51	17.035	0.175103	0.035819	615.9887	0.002244
4S	49.24389		104.0256	25.109	0.462504	0.240435	0.0000	0.083440
4P	42.02190		2326.556	27.884	0.468276	0.248714	806.7721	0.091233
4D	28.85679		11095.69	33.273	0.480255	0.266124	125.1573	0.112215
4F	11.28487		11820.08	42.037	0.514827	0.319643	26.1713	0.204839
5S	11.11525		44.47870	41.610	1.059617	1.252224	0.0000	2.232752
5P	8.553615		936.5848	45.122	1.149999	1.470481	130.0608	3.164861
6S	3.261942		18.77103	54.700	2.421492	6.494651	0.0000	58.592815
5D	4.892924		3799.978	52.380	1.401278	2.231272	14.3002	7.729051

Total Energy = -16801.216 Ry

Table I. (Continued)

	Ir^{+5}	$5d^2 6s^2$						
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5138.578	1341.612	0.725	0.019666	0.000517	0.0000	0.000001	
2S	868.0130	446.1359	4.606	0.082880	0.008052	0.0000	0.000109	
2P	832.5624	9519.828	5.722	0.070148	0.005959	16055.6778	0.000069	
3S	210.0266	210.9097	12.504	0.209316	0.049935	0.0000	0.003722	
3P	193.3722	4766.634	14.453	0.199849	0.046177	3490.4148	0.003321	
3D	162.7213	22024.30	17.034	0.175099	0.035818	616.0195	0.002244	
4S	50.53615	104.0458	25.100	0.462430	0.240752	0.0000	0.083367	
4P	43.31162	2326.867	27.876	0.468205	0.248628	8u6.9812	0.091141	
4D	30.14057	11096.61	33.267	0.480181	0.266009	125.1762	0.112222	
4F	12.56900	11836.21	41.967	0.513807	0.317978	26.2286	0.201261	
5S	12.30323	44.93645	41.327	1.051227	1.231203	0.0000	2.145257	
5P	9.696524	949.8066	44.764	1.132274	1.435633	133.7450	2.988621	
5D	6.012663	3932.695	51.684	1.362777	2.101401	15.2958	6.710587	
6S	4.096162	20.16544	53.543	2.302119	5.860013	0.0000	47.074886	

Total Energy = -16799.032 Ry

	Ir^{+6}	$5d^4 6s^2$						
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5139.971	1341.611	0.725	0.019666	0.000517	0.0000	0.000001	
2S	869.4118	446.1401	4.606	0.082879	0.008052	0.0000	0.000109	
2P	833.9615	9519.884	5.722	0.070147	0.005959	16055.9413	0.000069	
3S	211.4061	210.9210	12.502	0.209308	0.049931	0.0000	0.003721	
3P	194.7524	4766.886	14.450	0.199841	0.046173	3490.7815	0.003321	
3D	164.1030	22025.24	17.033	0.175095	0.035816	616.0604	0.002244	
4S	51.90091	104.0682	25.090	0.462342	0.240654	0.0000	0.083280	
4P	44.67369	2327.269	27.866	0.468112	0.248516	807.2487	0.091024	
4D	31.49598	11098.29	33.256	0.480063	0.265840	125.2094	0.111767	
4F	13.92451	11856.36	41.888	0.512644	0.316108	26.2977	0.197423	
5S	13.54499	45.42608	41.032	1.042581	1.209895	0.0000	2.059780	
5P	10.89102	963.7485	44.396	1.119500	1.401381	137.6839	2.823715	
5D	7.185096	4063.638	51.026	1.328248	1.989671	16.3084	5.913045	
6S	4.974855	21.46618	52.482	2.202471	5.358132	0.0000	38.973077	

Total Energy = -16796.069 Ry

Table I. (Continued)

Total Energy = -16792.476 Ry

Table I. (Continued)

Ir ⁺¹ 5d ⁶ 6s6p		<i>n</i>	<i>l</i>	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5133.958			1341.614		0.725	0.019666	0.000517	0.0000	0.000001
2S	863.378			446.1258		4.607	0.082881	0.008053	0.0000	0.000109
2P	827.9295			9519.713		5.723	0.070149	0.005960	16055.3379	0.000069
3S	205.4341			210.8773		12.511	0.209338	0.049946	0.0000	0.003724
3P	188.7812			4766.031		14.459	0.199870	0.046187	3489.5726	0.003323
3D	158.1299			22022.55		17.037	0.175108	0.035821	615.9483	0.002245
4S	45.96774			103.9777		25.127	0.462664	0.241011	0.0000	0.083590
4P	38.75534			2326.176		27.894	0.468373	0.248832	806.5235	0.091372
4D	25.60375			11096.63		33.277	0.480295	0.266221	125.1770	0.112479
4F	8.030071			11791.00		42.174	0.516855	0.323124	26.0683	0.213228
5S	8.039358			43.28149		42.380	1.083175	1.313231	0.0000	2.507924
5P	5.602136			904.1311		46.043	1.179050	1.567437	121.2368	3.703244
5D	2.004201			3405.667		54.692	1.546503	2.777301	11.5306	13.302906
6S	1.193820			14.00217		58.930	2.988331	10.036016	0.0000	151.657185
6P	0.795864			241.7715		62.635	3.689418	15.343892	8.6753	360.399641

Total Energy = -16805.436 Ry

Ir ⁺² 5d ⁵ 6s6p		<i>n</i>	<i>l</i>	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5134.975			1341.613		0.725	0.019666	0.000517	0.0000	0.000001
2S	864.3988			446.126		4.607	0.082881	0.008053	0.0000	0.000109
2P	828.9498			9519.726		5.723	0.070149	0.005960	16055.3861	0.000069
3S	206.4490			210.881		12.510	0.209336	0.049945	0.0000	0.003724
3P	189.7963			4766.140		14.458	0.199866	0.046185	3489.7234	0.003322
3D	159.1439			22022.70		17.037	0.175107	0.035821	615.9550	0.002245
4S	46.98023			103.9860		25.124	0.462641	0.249984	0.0000	0.083566
4P	39.76670			2326.295		27.891	0.468346	0.248801	806.5991	0.091337
4D	26.61117			11095.93		33.278	0.480309	0.266224	125.1637	0.112438
4F	9.036143			11797.82		42.139	0.516337	0.322203	26.0926	0.210827
5S	9.000173			43.59857		42.167	1.076565	1.295768	0.0000	2.425796
5P	6.529209			914.2874		45.741	1.16/667	1.534198	123.9637	3.507908
5D	2.909275			3541.791		53.838	1.489538	2.551749	12.4548	10.721571
6S	1.861139			15.85209		57.248	2.733967	8.333593	0.0000	100.380921
6P	1.389673			296.4973		60.499	3.211934	11.509500	13.0372	192.74247

Total Energy = -16804.515 Ry

Table I. (Continued)

$\text{Ir}^{+3} \quad 5d^4 \quad 6s6p$		$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5136.095		1341.612		0.725	0.019666	0.000517	0.0000	0.000001
2S	665.5302		446.1281		4.607	0.082881	0.008053	0.0000	0.000109
2P	830.0808		9519.728		5.723	0.070149	0.005960	16055.4083	0.000069
3S	207.5729		210.8871		12.509	0.209332	0.049943	0.0000	0.003723
3P	190.9206		4766.262		14.457	0.199863	0.046183	3489.9197	0.003322
3D	160.2683		22022.95		17.036	0.175106	0.035820	615.96/2	0.002245
4S	48.09930		103.9962		25.120	0.462609	0.240947	0.0000	0.083531
4P	40.88444		2326.473		27.887	0.468303	0.248752	806.7124	0.091284
4D	27.72415		11095.59		33.277	0.480298	0.266193	125.15/2	0.112352
4F	10.151569		11807.56		42.093	0.515651	0.321024	26.1273	0.207975
5S	10.04973		43.96475		41.928	1.069244	1.276774	0.0000	2.339999
5P	7.541050		925.7052		45.414	1.155581	1.499748	127.0693	3.316721
5D	3.897652		3676.973		53.052	1.440620	2.370021	13.4060	8.937212
6S	2.593722		17.50174		55.825	2.550161	7.219405	0.0000	73.445529
6P	2.054312		342.5259		58.809	2.913484	9.424252	17.3900	125.580161

Total Energy = -16803.104 Ry

$\text{Ir}^{+4} \quad 5d^3 \quad 6s6p$		$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5137.324		1341.612		0.725	0.019666	0.000517	0.0000	0.000001
2S	866.7603		446.1313		4.607	0.082880	0.008053	0.0000	0.000109
2P	831.3112		9519.784		5.722	0.070148	0.005960	16055.5985	0.000069
3S	208.7901		210.8952		12.507	0.209326	0.049940	0.0000	0.003723
3P	192.1384		4766.453		14.455	0.199855	0.046180	3490.1612	0.003322
3D	161.4865		22023.49		17.035	0.175103	0.035819	615.9891	0.002244
4S	49.30831		104.0100		25.115	0.462558	0.240890	0.0000	0.083480
4P	42.09189		2326.721		27.881	0.468250	0.248886	806.8827	0.091212
4D	28.92634		11095.91		33.272	0.480246	0.266115	125.1621	0.112208
4F	11.17117		11820.58		42.035	0.514794	0.319593	26.1732	0.204726
5S	11.17117		44.37324		41.670	1.061421	1.256782	0.0000	2.253019
5P	8.621504		938.1599		45.069	1.143103	1.464962	130.4994	3.133711
5D	4.954284		3810.617		52.320	1.397880	2.219548	14.3794	7.634570
6S	3.381485		19.00580		54.568	2.407290	6.417185	0.0000	57.042959
6P	2.778576		383.1380		57.368	2.699676	8.071956	21.7493	90.443919

Total Energy = -16801.216 Ry

Table I. (Continued)

Ir ⁺⁵ 5d ² 6s6p		$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5138.633	1341.611	0.725	0.019666	0.000517	0.00000	0.000001	
2S	668.0743	444.1335	4.606	0.002880	0.008053	0.00000	0.000109	
2P	832.6253	9519.825	5.722	0.070148	0.005959	16055.7870	0.000069	
3S	210.0893	210.9040	12.505	0.209320	0.049937	0.00000	0.003722	
3P	193.4381	4764.657	14.453	0.199849	0.046177	3490.4721	0.003321	
3D	162.7870	22024.18	17.034	0.175100	0.035818	616.0216	0.002244	
4S	50.59658	104.0266	25.107	0.462493	0.240818	0.00000	0.083414	
4P	43.37839	2327.050	27.8/3	0.468177	0.245597	807.1041	0.091118	
4D	30.20677	11094.82	33.266	0.480171	0.265998	125.1812	0.112013	
4F	12.63544	11834.87	41.966	0.513789	0.317939	26.2305	0.201157	
5S	12.35452	44.81952	41.394	1.053179	1.236087	0.00000	2.166314	
5P	9.760764	951.4527	44.711	1.130424	1.430408	134.2035	2.960969	
5D	6.070264	3942.599	51.631	1.359940	2.092658	15.3713	6.642602	
6S	4.21878	27.39549	53.430	2.291089	5.803998	0.00000	46.092600	
6P	3.555458	419.9431	56.091	2.534760	7.106886	26.1179	69.227223	
Total Energy = -16798.764 Ry								
Ir ⁺⁶ 5d ¹ 6s6p		$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5140.026	1341.610	0.725	0.019666	0.000517	0.00000	0.000001	
2S	669.4703	444.1372	4.606	0.002879	0.008052	0.00000	0.000109	
2P	834.0221	9519.881	5.721	0.070147	0.005959	16055.8830	0.000069	
3S	211.4653	210.9150	12.503	0.209311	0.049933	0.00000	0.003722	
3P	194.8154	4764.937	14.449	0.199838	0.046172	3490.8309	0.003320	
3D	164.1656	22125.10	17.033	0.175095	0.035816	616.0569	0.002244	
4S	51.95783	104.0490	25.098	0.462408	0.240723	0.00000	0.083329	
4P	44.73773	2327.500	27.863	0.468078	0.248479	807.4166	0.090997	
4D	31.55931	11795.57	33.255	0.480051	0.265826	125.2165	0.111755	
4F	13.98766	11554.78	41.886	0.512614	0.316056	26.2997	0.197303	
5S	13.59144	45.29783	41.104	1.044674	1.215057	0.00000	2.081312	
5P	10.95213	965.4228	44.344	1.117726	1.396508	138.1590	2.799403	
5D	7.239522	4072.872	50.979	1.325842	1.982061	16.3416	5.862355	
6S	5.099189	21.69900	52.381	2.193400	5.315075	0.00000	38.303345	
6P	4.380128	453.9546	54.930	2.401403	6.374983	30.5084	55.197452	
Total Energy = -16795.752 Ry								

Table I. (Continued)

$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5141.502	1341.610	0.725	0.019666	0.000517	0.0000	0.000001
2S	870.9434	446.1426	4.605	0.082878	0.008052	0.0000	0.000109
2P	835.4963	9519.981	5.721	0.070146	0.005959	16056.1989	0.000069
3S	212.9134	210.9284	12.499	0.209301	0.049928	0.0000	0.003721
3P	196.2649	4767.274	14.446	0.199826	0.046167	3491.2833	0.003320
3D	165.6169	22026.32	17.031	0.175089	0.035813	616.1039	0.002244
4S	53.38658	104.0719	25.087	0.462312	0.240614	0.0000	0.083229
4P	46.16435	2328.035	27.851	0.467960	0.248338	807.7663	0.090852
4D	32.97843	11101.12	33.240	0.479889	0.265602	125.2673	0.111436
4F	15.40677	11880.32	41.795	0.511291	0.313976	26.3809	0.193235
5S	14.87797	45.80458	40.803	1.035990	1.193911	0.0000	1.998757
5P	12.19059	979.9592	43.971	1.105092	1.363451	142.3308	2.648818
6S	6.021534	22.92858	51.400	2.109411	4.913547	0.0000	32.507223
6P	5.246586	485.7639	53.157	2.290084	5.796486	34.9218	45.325570

Total Energy = -16792.166 Ry

nl	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5133.391	1341.614	0.125	0.019666	0.000517	0.0000	0.0000001
2S	862.8138	446.1264	4.607	0.082881	0.008053	0.0000	0.000109
2P	827.3641	9519.705	5.723	0.070149	0.005960	16055.3137	0.000069
3S	204.8702	210.8796	12.511	0.209336	0.049945	0.0000	0.003724
3P	188.2163	4766.034	14.459	0.199870	0.046186	3489.5835	0.003323
3D	157.5640	22022.51	17.037	0.175109	0.035821	615.9513	0.002245
4S	45.40497	103.9846	25.124	0.462645	0.240991	0.0000	0.083575
4P	38.19058	2326.137	27.894	0.468375	0.248837	806.4864	0.091377
4D	25.03840	11096.32	33.278	0.480310	0.266235	125.1718	0.112487
4F	7.464959	11790.83	42.174	0.516862	0.323131	26.0674	0.213249
5S	7.480402	43.34159	42.345	1.082088	1.310432	0.0000	2.494923
5P	5.037116	903.5210	46.078	1.180396	1.572103	121.0732	3.742428
6S	0.661244	12.77514	60.198	3.213857	11.776217	0.0000	223.456865
5D	1.444467	3381.017	54.911	1.561831	2.846320	11.3661	14.350899
6P	0.367474	207.0434	64.345	4.187996	20.207178	6.3648	685.512971

Total Energy = -16805.768 Ry

Table I. (Continued)

	Ir^{+1}	$5d^5 6s^2 6p$						
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5134.309	1341.614	0.725	0.019666	0.000517	0.0000	0.000001	
2S	863.7330	446.1270	4.607	0.082881	0.008053	0.0000	0.000109	
2P	828.2830	9519.718	5.723	0.070149	0.005960	16055.3177	0.00069	
3S	205.7839	210.8845	12.509	0.209333	0.049944	0.0000	0.003723	
3P	189.1297	4766.107	14.459	0.199868	0.046186	3489.7033	0.003322	
3D	158.4770	22022.64	17.037	0.175108	0.035821	615.9492	0.002245	
4S	46.31686	103.9938	25.122	0.462621	0.240962	0.0000	0.083550	
4P	39.10059	2326.196	27.893	0.468362	0.248820	806.5291	0.091353	
4D	25.94439	11095.30	33.280	0.480330	0.266250	125.1494	0.112461	
4F	8.371747	11796.82	42.142	0.516388	0.322287	26.0886	0.211014	
5S	8.346589	43.66498	42.131	1.075444	1.292932	0.0000	2.413171	
5P	5.868923	913.0700	45.797	1.169757	1.540977	123.6383	3.557585	
6S	1.256247	14.72775	58.250	2.880016	9.315620	0.0000	130.222012	
5D	2.257789	3510.372	54.080	1.505237	2.616492	12.2380	11.518622	
6P	0.895686	270.9498	61.607	3.443013	13.342693	10.8909	270.074867	
Total Energy = -16805.128 Ry								

	Ir^{+2}	$5d^4 6s^2 6p$						
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5135.349	1341.612	0.725	0.019666	0.000517	0.0000	0.000001	
2S	84.7832	446.1292	4.607	0.082881	0.008053	0.0000	0.000109	
2P	829.3324	9519.726	5.723	0.070149	0.005960	16055.3898	0.00069	
3S	206.8276	210.8908	12.508	0.209329	0.049942	0.0000	0.003723	
3P	190.1733	4766.255	14.457	0.199861	0.046183	3489.8833	0.003322	
3D	159.5202	22022.80	17.037	0.175107	0.035821	615.9640	0.002245	
4S	47.35739	104.0068	25.117	0.462579	0.240917	0.0000	0.083511	
4P	40.13902	2326.348	27.890	0.468332	0.248781	806.6378	0.091308	
4D	26.97821	11094.77	33.280	0.480325	0.266229	125.1387	0.112388	
4F	9.406308	11805.22	42.101	0.515781	0.321224	26.1190	0.208377	
5S	9.325189	44.03151	41.894	1.068185	1.274132	0.0000	2.328617	
5P	6.809579	923.8339	45.488	1.158303	1.508190	126.5577	3.372550	
6S	1.933629	16.44847	56.672	2.656375	7.865400	0.0000	89.277270	
5D	3.177721	3640.877	53.300	1.455703	2.427981	13.1483	9.542952	
6P	1.508949	321.3315	59.670	3.058267	10.433831	15.3116	157.753207	
Total Energy = -16804.066 Ry								

Table I. (Continued)

Total Energy = -16802.547 Ry

nl	$\epsilon_{nl, nl}$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5131.748	1341.611	0.725	0.019666	0.000017	0.00000	0.000001
2S	861.1940	446.1343	4.606	0.082880	0.008052	0.0000	0.000109
2P	831.7427	9519.789	5.722	0.070148	0.005960	16055.5873	0.000069
3S	209.2135	210.9980	12.534	0.209316	0.049936	0.0000	0.003722
3P	192.5597	4766.631	14.452	0.199848	0.046177	3490.4069	0.003321
3D	161.9172	22023.81	17.035	0.175101	0.035818	616.0074	0.002244
4S	49.72739	104.0401	25.103	0.462458	0.240782	0.0000	0.083395
4P	42.50445	7326.851	27.877	0.468217	0.248643	806.9728	0.091159
4D	29.33216	11095.23	33.272	0.480237	0.266079	125.1487	0.112098
4F	11.76132	11831.90	41.984	0.514048	0.318341	26.2129	0.201925
5S	11.51808	44.68263	41.364	1.052312	1.233991	0.0000	2.15/829
5P	8.917691	948.4030	44.815	1.134069	1.440950	133.3517	3.020661
6S	3.469394	19.42533	54.111	2.359238	6.162200	0.0000	5.564807
5D	5.242761	3900.558	51.880	1.373405	2.138455	15.0517	7.021170
6P	2.927690	403.3232	56.728	2.614442	7.575421	24.0954	79.587227

Total Energy = -16800.504 Ry

Table I. (Continued)

Ir ⁺⁵ 5d ¹ 6s ² 6p		ϵ_{nl}	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5139.080		1341.610	0.725	0.019666	0.000517	0.0000	0.000001
2S	868.5311		446.1374	4.606	0.082880	0.008052	0.0000	0.000109
2P	833.0801		9519.838	5.722	0.070148	0.005959	16055.7565	0.00069
3S	210.5326		210.9179	12.503	0.209311	0.049933	0.0000	0.003722
3P	193.8795		4766.856	14.451	0.199842	0.046173	3491.7449	0.003321
3D	163.2282		22024.68	17.033	0.175097	0.035817	616.0432	0.002244
4S	51.03350		104.0618	25.094	0.462374	0.240692	0.0000	0.083313
4P	43.80802		2327.230	27.869	0.468132	0.248541	807.2266	0.091051
4D	30.62897		11096.49	33.262	0.480136	0.265932	125.1730	0.111867
4F	13.05838		11850.23	41.909	0.512955	0.316574	26.2767	0.198253
5S	12.70862		45.35778	41.077	1.043908	1.213239	0.0000	2.074176
5P	10.06216		961.8832	44.459	1.121662	1.407590	137.1518	2.858381
6S	4.312454		20.75316	53.013	2.251226	5.602127	0.0000	42.913589
5D	6.386447		4028.887	51.225	1.338524	2.023914	16.0367	6.172881
6P	3.716955		438.6868	55.506	2.465757	6.730392	28.4949	62.072719
Total Energy = -16797.922 Ry								

Ir ⁺⁶ 5d ⁰ 6s ² 6p		ϵ_{nl}	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5140.494		1341.609	0.725	0.019666	0.000517	0.0000	0.000001
2S	869.9467		446.1431	4.605	0.082878	0.008052	0.0000	0.000109
2P	834.4961		9519.925	5.721	0.070147	0.005959	16056.0634	0.00069
3S	211.9261		210.9320	12.499	0.209299	0.049928	0.0000	0.003721
3P	195.2738		4767.186	14.447	0.199830	0.046168	3491.1865	0.003320
3D	164.6240		22025.71	17.031	0.175092	0.035814	616.0842	0.002244
4S	52.41022		104.0868	25.083	0.462279	0.240584	0.0000	0.083216
4P	45.18205		2327.690	27.858	0.468029	0.248416	807.5404	0.090920
4D	31.99533		11098.59	33.250	0.480000	0.265736	125.2167	0.111576
4F	14.42523		11872.15	41.824	0.511709	0.314599	26.3526	0.194338
5S	13.95213		45.86112	40.780	1.055327	1.192358	0.0000	1.992820
5P	11.25772		975.9/57	44.095	1.109271	1.374896	141.1832	2.706319
6S	5.199493		22.00152	51.996	2.129622	5.150665	0.0000	35.944177
6P	4.252791		471.515/	54.387	2.343833	6.077796	32.9050	50.179573
Total Energy = -16794.791 Ry								

Table I. (Continued)

Total Energy = -16805.591 Ry

Table I. (Continued)

	Ir^{+2}	$5d^4 6s6p^2$						
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5135.419	1341.611	0.725	0.019666	0.000517	0.0000	0.000001	
2S	864.8593	446.1272	4.607	0.082881	0.008053	0.0000	0.000109	
2P	829.4095	9519.712	5.723	0.070149	0.005960	16055.5712	0.000069	
3S	206.9047	210.8868	12.509	0.209332	0.049943	0.0000	0.003723	
3P	190.2527	4766.268	14.457	0.199861	0.046183	3489.9048	0.003322	
3D	159.5995	22022.71	17.036	0.175106	0.035821	615.9588	0.002245	
4S	47.43295	103.9937	25.121	0.462616	0.240959	0.0000	0.083543	
4P	40.21832	2326.483	27.887	0.468308	0.248757	806.7249	0.091290	
4D	27.05774	11094.90	33.280	0.480324	0.266226	125.1435	0.112385	
4F	9.485734	11805.69	42.099	0.515749	0.321180	20.123	0.208277	
5S	9.393744	43.94801	41.941	1.069634	1.277852	0.0000	2.345829	
5P	6.887315	925.2270	45.438	1.156436	1.502513	126.9400	3.337154	
5D	3.249595	3653.261	53.223	1.450954	2.410351	15.2366	9.374122	
6S	2.051331	16.71487	56.482	2.631857	7.113647	0.0000	85.387074	
6P	1.497806	319.8490	59.665	3.057324	10.427289	15.1674	157.726764	
Total Energy = -16803.824 Ry								

	Ir^{+3}	$5d^3 6s6p^2$						
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5136.572	1341.611	0.725	0.019666	0.000517	0.0000	0.000001	
2S	866.0141	446.1295	4.607	0.082881	0.008053	0.0000	0.000109	
2P	830.5644	9519.754	5.723	0.070149	0.005960	16055.5108	0.000069	
3S	206.0476	210.8937	12.508	0.209327	0.049941	0.0000	0.003723	
3P	191.3962	4766.442	14.455	0.199855	0.046180	3490.1456	0.003322	
3D	160.7431	22023.15	17.036	0.175105	0.035820	615.9804	0.002244	
4S	46.56896	104.0074	25.116	0.462570	0.240907	0.0000	0.083496	
4P	41.35349	2326.715	27.882	0.468256	0.248695	806.8761	0.091224	
4D	28.18681	11094.95	33.276	0.480289	0.266166	125.1440	0.112261	
4F	10.61534	11817.28	42.047	0.514973	0.319860	26.1619	0.205220	
5S	10.44889	44.34312	41.692	1.062074	1.258542	0.0000	2.261773	
5P	7.903301	937.2078	45.106	1.144432	1.469047	130.2345	3.160271	
5D	4.243353	3782.547	52.503	1.408333	2.257858	14.1719	7.994441	
6S	2.794174	18.24475	55.168	2.473389	6.787295	0.0000	64.625844	
6P	2.172759	362.5193	58.105	2.804943	8.737985	19.4745	107.810119	
Total Energy = -16802.281 Ry								

Table I. (Continued)

		Ir^{+4}	$5d^2 6s6p^2$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
$n\ell$	$\epsilon_{nl, nl}$								
1S	5137.815		1341.610	0.725	0.019666	0.000517	0.00000	0.000001	
2S	867.2624		446.1317	4.607	0.082881	0.008053	0.00000	0.000109	
2P	831.8130		9519.791	5.722	0.070148	0.005960	16055.6090	0.000069	
3S	209.2819		210.9026	12.506	0.209320	0.049938	0.00000	0.003722	
3P	192.6313		4766.662	14.452	0.199848	0.046176	3490.4528	0.003321	
3D	161.9787		22023.72	17.035	0.175102	0.035819	616.6018	0.002244	
4S	49.79337		104.0223	25.110	0.462518	0.240845	0.00000	0.083438	
4P	42.57633		2327.016	27.875	0.468193	0.248616	8.7.0472	0.091138	
4D	29.40354		11095.43	33.271	0.480229	0.266069	125.1535	0.112089	
4F	11.83249		11832.59	41.981	0.514009	0.318281	26.2151	0.201794	
5S	11.57408		44.77491	41.426	1.054129	1.238546	0.0000	2.177711	
5P	8.986191		950.0448	44.761	1.132181	1.435585	133.8107	2.991667	
5D	5.304527		3911.198	51.822	1.370220	2.127836	15.1323	6.941458	
6S	3.591327		19.66066	53.987	2.346478	6.094897	0.0000	51.298080	
6P	2.906223		400.8493	56.749	2.61/142	7.589296	23.8008	79.908598	

Total Energy = -16800.215 Ry

		Ir^{+5}	$5d^1 6s6p^2$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
$n\ell$	$\epsilon_{nl, nl}$								
1S	5139.148		1341.610	0.725	0.019666	0.000517	0.00000	0.000001	
2S	868.5960		446.1353	4.606	0.082880	0.008052	0.00000	0.000109	
2P	833.1476		9519.655	5.721	0.070147	0.005959	16055.7644	0.000069	
3S	210.5972		210.9131	12.503	0.209313	0.049934	0.00000	0.003722	
3P	193.9477		4766.923	14.450	0.199839	0.046172	3490.8105	0.003321	
3D	163.2960		22024.59	17.033	0.175097	0.035817	616.0391	0.002244	
4S	51.09532		104.0422	25.101	0.462440	0.240759	0.00000	0.083361	
4P	43.87655		2327.441	27.865	0.468099	0.248505	807.3666	0.091025	
4D	30.69684		11096.80	33.261	0.480123	0.265947	125.1803	0.111653	
4F	18.12607		11850.93	41.906	0.512912	0.316508	26.2793	0.198112	
5S	12.75969		45.23872	41.145	1.045867	1.218103	0.00000	2.094758	
5P	10.12690		963.5766	44.406	1.119849	1.402558	137.6327	2.832697	
5D	6.424631		4038.737	51.174	1.335871	2.015390	16.1139	6.113955	
6S	4.436707		20.98645	52.904	2.241004	5.551869	0.00000	42.080885	
6P	3.691422		436.0030	55.532	2.468626	6.745104	28.1482	62.351905	

Total Energy = -16797.606 Ry

Table I. (Continued)

	Ir^{+6}	$5d^0 6s^2 6p^2$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5140.551	1341.608	0.726	0.019666	0.000517	0.0000	0.000001	
2S	870.0075	445.1394	4.606	0.082879	0.008052	0.0000	0.000109	
2P	634.5593	9519.914	5.721	0.070147	0.005959	16056.0797	0.000069	
3S	211.9875	211.9245	12.501	0.209305	0.049930	0.0000	0.003721	
3P	195.3395	4767.213	14.447	0.199830	0.046168	3491.2313	0.003320	
3D	164.6895	22125.61	17.031	0.175092	0.035814	616.0793	0.002244	
4S	52.46918	104.0651	25.191	0.462349	0.240657	0.0000	0.083268	
4P	45.24833	2327.939	27.854	0.467992	0.248375	807.7163	0.090890	
4D	32.06114	11.98.86	33.249	0.479986	0.265720	125.2228	0.11562	
4F	14.49044	11.87.86	41.820	0.511662	0.314526	26.3554	0.194189	
5S	13.99896	45.73106	40.852	1.037410	1.197468	0.0000	2.013769	
5P	11.31942	977.6883	44.044	1.107539	1.370209	141.6760	2.683656	
6S	5.326144	22.23811	51.897	2.151102	5.111361	0.0000	35.363139	
6P	4.523621	468.7375	54.418	2.346991	6.092021	32.5223	50.411314	
Total Energy = -16794.435 Ry								

	Ir^0	$5d^5 6s^2 6p^2$	a_{nl}	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5133.798	1341.613	0.725	0.019666	0.000517	0.0000	0.000001	
2S	863.2278	446.1271	4.607	0.082881	0.008053	0.0000	0.000109	
2P	827.7777	9519.708	5.723	0.070149	0.005960	16055.3603	0.000069	
3S	205.2800	210.8836	12.510	0.209335	0.049944	0.0000	0.003723	
3P	188.6263	4766.130	14.458	0.199867	0.046185	3489.7276	0.003322	
3D	157.9733	22022.54	17.037	0.175108	0.035821	615.9492	0.002245	
4S	45.81359	103.9923	25.122	0.462627	0.240970	0.0000	0.083557	
4P	38.59811	2326.239	27.892	0.468358	0.248815	806.5611	0.091350	
4D	22.44148	11095.18	33.281	0.480338	0.266257	125.1487	0.112467	
4F	7.869006	11796.32	42.144	0.516413	0.32322	26.0871	0.211071	
5S	7.845046	43.65579	42.136	1.075609	1.293366	0.0000	2.415487	
5P	5.369169	913.2761	45.794	1.169642	1.540819	123.6948	3.560344	
6S	0.819693	13.95476	59.057	3.009503	10.265441	0.0000	165.448657	
5D	1.75861	3499.753	54.181	1.511892	2.646337	12.1647	11.967745	
6P	0.4472/3	242.2506	62.943	3.770399	16.280416	8.7086	434.961606	
Total Energy = -16803.319 Ry								

Table I. (Continued)

$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5134.739	1341.612	0.725	0.019666	0.000517	0.0000	0.000001
2S	864.1758	446.1283	4.607	0.082881	0.008053	0.0000	0.000109
2P	828.7250	9519.719	5.723	0.070149	0.005960	16055.3579	0.00069
3S	206.2210	210.8898	12.508	0.209329	0.049942	0.0000	0.003723
3P	189.5673	4766.201	14.457	0.199861	0.046183	3489.8880	0.003322
3D	158.9137	22022.68	17.036	0.175106	0.035821	615.9567	0.002245
4S	46.75163	104.0042	25.118	0.462588	0.240929	0.0000	0.083522
4P	39.53429	2362.379	27.889	0.468329	0.248780	806.6569	0.091309
4D	26.37280	11094.32	33.281	0.480346	0.266253	125.1304	0.112411
4F	8.801180	11804.08	42.105	0.515839	0.321312	26.1152	0.208548
5S	8.725789	44.01328	41.906	1.068553	1.275114	0.0000	2.333622
5P	6.213017	923.7091	45.499	1.158679	1.509548	126.5240	3.385012
6S	1.43.3/5	15.6/464	57.378	2.752057	8.485241	0.0000	106.711425
5D	2.584226	3622.958	53.440	1.464368	2.463167	13.0212	5.964012
6P	-0.95555	297.1464	60.447	3.246985	11.090917	13.0956	21.149981

Total Energy = -16804.560 Ry

$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5135.804	1341.611	0.725	0.019666	0.000517	0.0000	0.000001
2S	865.2497	446.1305	4.607	0.082881	0.008053	0.0000	0.000109
2P	829.7982	9519.734	5.723	0.070149	0.005960	16055.4559	0.00069
3S	207.2863	210.8963	12.508	0.209327	0.049940	0.0000	0.003723
3P	190.6328	4766.426	14.455	0.199856	0.046180	3490.1305	0.003322
3D	159.9790	22022.97	17.036	0.175105	0.035820	615.9718	0.002244
4S	47.81221	104.0184	25.113	0.462541	0.240877	0.0000	0.083477
4P	40.59292	2326.569	27.885	0.468287	0.248728	806.7862	0.091252
4D	27.42573	11093.93	33.280	0.480329	0.266214	125.1232	0.112310
4F	9.855059	11814.59	42.057	0.515121	0.320090	26.1522	0.205679
5S	9.712620	44.40899	41.657	1.061030	1.255955	0.0000	2.250646
5P	7.159935	935.1122	45.184	1.147215	1.477446	129.6539	3.212741
6S	2.120134	17.24736	55.949	2.565180	7.325833	0.0000	76.899352
5D	3.511585	3747.905	52.730	1.421531	2.306776	15.917	8.468216
6P	1.615988	343.0680	58.897	2.927758	9.561697	1/.4490	132.082338

Total Energy = -16803.319 Ry

Table I. (Continued)

	Ir^{+3}	$5d^2 6s^2 6p^2$						
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5136.971	1341.610	0.725	0.019666	0.000517	0.0000	0.000001	
2S	866.4281	446.1333	4.606	0.082880	0.008053	0.0000	0.000109	
2P	830.9762	9519.758	5.722	0.070148	0.005960	16055.5978	0.000069	
3S	208.4533	210.9069	12.505	0.209317	0.049936	0.0000	0.003722	
3P	191.8000	4766.634	14.453	0.199848	0.046177	3490.4244	0.003321	
3D	161.1463	22023.36	17.035	0.175103	0.035819	615.9945	0.002244	
4S	48.97094	104.0357	25.106	0.462483	0.240812	0.0000	0.083418	
4P	41.74944	2326.845	27.878	0.468225	0.248654	806.9712	0.091172	
4D	28.57615	11194.20	33.275	0.480279	0.266132	125.1287	0.112155	
4F	11.00590	11828.28	41.997	0.514235	0.318626	26.2001	0.202450	
5S	10.78008	44.83875	41.393	1.053172	1.236212	0.0000	2.167965	
5P	8.184921	947.3930	44.853	1.135417	1.445022	133.0684	3.046421	
6S	2.871683	18.69638	54.690	2.420411	6.498178	0.0000	59.179021	
5D	4.516993	3873.142	52.054	1.382984	2.172696	14.8446	7.326740	
6P	2.307020	383.5382	57.429	2.708132	8.148634	21.7932	93.564502	
Total Energy = -16801.629 Ry								

	Ir^{+4}	$5d^1 6s^2 6p^2$						
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$	
1S	5138.240	1341.609	0.725	0.019666	0.000517	0.0000	0.000001	
2S	667.7004	446.1361	4.606	0.082880	0.008052	0.0000	0.000109	
2P	632.2485	9519.806	5.722	0.070148	0.005959	16055.7292	0.000069	
3S	209.7084	210.9163	12.503	0.209312	0.049933	0.0000	0.003722	
3P	193.0558	4766.855	14.451	0.199842	0.046173	3490.7484	0.003321	
3D	162.4029	22024.15	17.034	0.175099	0.035817	616.0235	0.002244	
4S	50.21417	104.0555	25.098	0.462407	0.240728	0.0000	0.083344	
4P	42.99031	2327.202	27.870	0.468145	0.248559	807.2088	0.091071	
4D	29.81038	11095.03	33.268	0.480197	0.266008	125.1447	0.111949	
4F	12.24027	11845.25	41.927	0.513208	0.316955	26.2596	0.198937	
5S	11.91482	45.30098	41.115	1.045006	1.216023	0.0000	2.086305	
5P	9.274846	960.4194	44.510	1.123429	1.412710	136.7369	2.887961	
5D	5.587447	3998.129	51.408	1.348069	2.056386	15.7976	6.431860	
6S	3.676379	20.04699	53.552	2.312938	5.869270	0.0000	47.533074	
6P	3.054379	421.2203	56.138	2.540512	7.155837	26.1511	70.973947	
Total Energy = -16799.440 Ry								

Table I. (Continued)

Ir^{+5}	$5d$	0	2	$6s$	2	$6p$	
$n\ell$	$\epsilon_{n\ell, n\ell}$	$a_{n\ell}$	σ	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r^3 \rangle$	$\langle r^4 \rangle$
1S	5139.592	1341.609	0.725	0.019666	0.000517	0.0000	0.000001
2S	869.0548	446.1403	4.605	0.082879	0.008052	0.0000	0.000109
2P	833.6034	9519.876	5.721	0.070147	0.005959	16055.9474	0.000069
3S	211.0424	210.9286	12.500	0.209302	0.049929	0.0000	0.003721
3P	194.3906	4767.147	14.447	0.199832	0.046169	3491.1466	0.003320
3D	163.7388	22025.10	17.032	0.175094	0.035815	616.0648	0.002244
4S	51.53322	104.0795	25.088	0.462317	0.240626	0.0000	0.083253
4P	44.30689	2327.665	27.859	0.468442	0.248437	807.5169	0.090946
4D	31.11906	11096.72	33.257	0.480075	0.265831	125.1792	0.111681
4F	13.54959	11865.49	41.846	0.512037	0.315086	26.3300	0.195183
5S	13.10819	45.79025	40.825	1.036437	1.195636	0.0000	2.006532
5P	10.42139	974.0699	44.157	1.111364	1.380816	140.6324	2.738256
6S	4.528521	21.31583	52.504	2.204440	5.370255	0.0000	39.341852
6P	3.851993	454.0994	54.970	2.405804	6.409696	30.5267	56.288112

III. ENERGY LEVELS

Figure 1 illustrates the effect on the one-electron energies $\epsilon_{nl, nl}$ of changing the configuration and holding the ionization state constant. It is observed that the shell energies below 4d remain constant independent of N, M, and K. The 4f and 5s levels are almost degenerate.

Figure 2 shows the effect of changing the ionization state of the $5d^N 6s6p$ configuration by reducing N. Each nl level becomes more tightly bound as N decreases, the effect being fractionally larger for the outer shells.

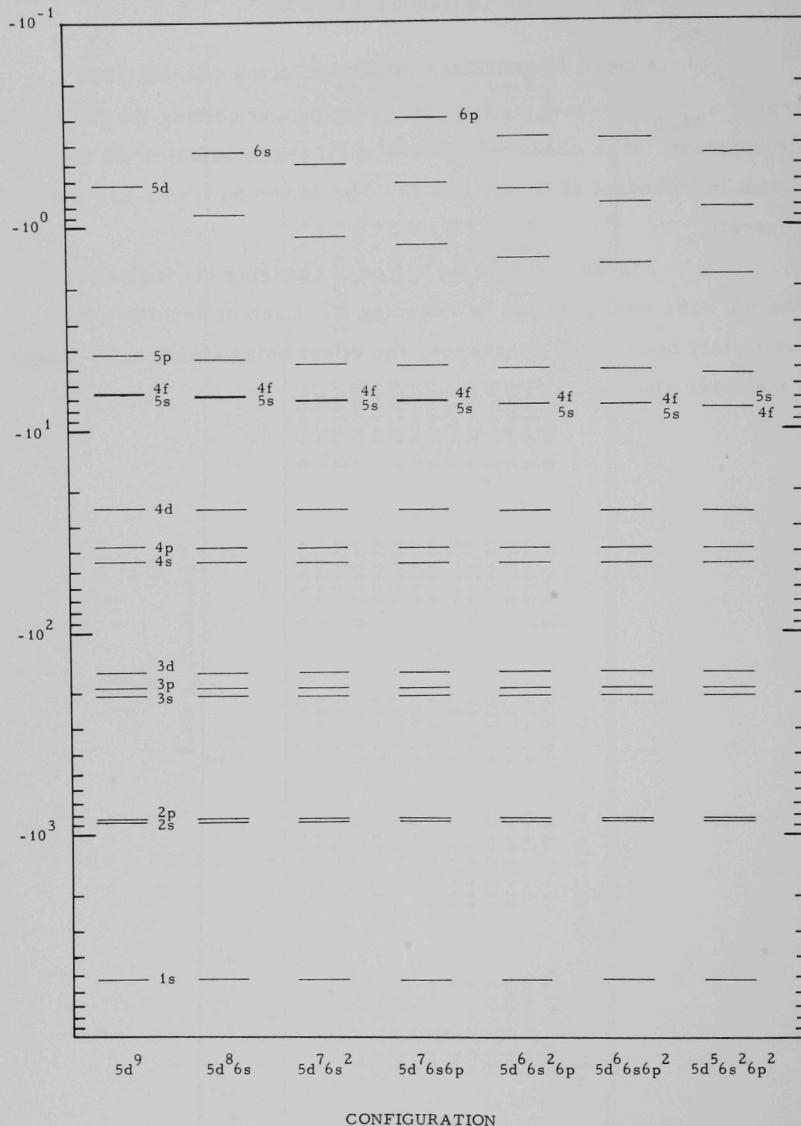
ENERGY PARAMETER - $\epsilon_{nl, n\ell}$ (Ry)

Fig. 1. One-electron energies $\epsilon_{nl, n\ell}$ vs outer electron configuration for the neutral atom Ir⁰.

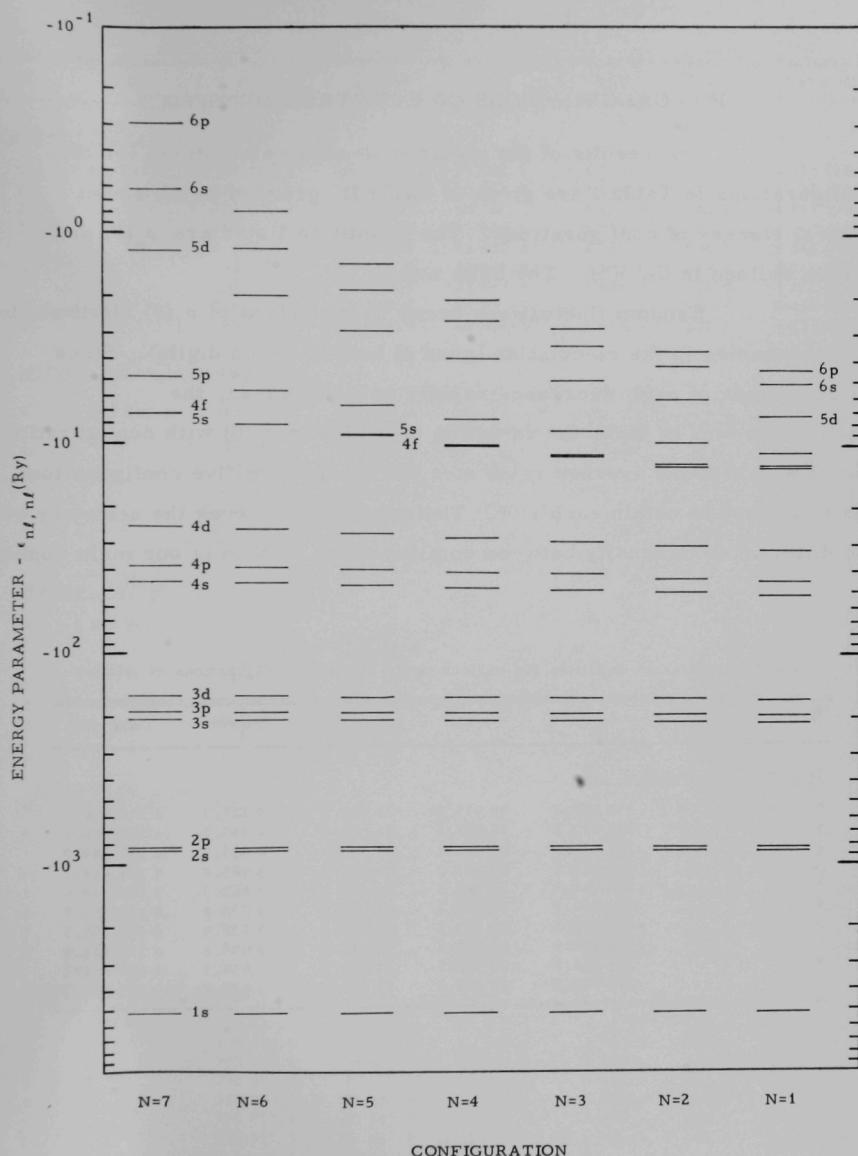


Fig. 2. One-electron energies $\epsilon_{nl, nl}$ vs ionization state for the $5d^N 6s 6p$ configuration.

IV. CALCULATIONS OF ELECTRON DENSITIES

The results of the electron-density calculations for the configurations in Table I are given in Table II, grouped in the seven general classes of configurations. The quantities listed are $\rho_n(0)$ and $\rho(0)$ as defined in Eq. (5). The units are a_0^{-3} .

Random fluctuations occur in the values of $\rho_1(0)$ attributable to inaccuracies in the calculation (good at best to seven digits). Since the magnitude of $\rho_n(0)$ decreases rapidly as n increases, the fluctuations tend to mask the variation of $\rho_5(0)$ and $\rho_6(0)$ with configuration. For this reason the average value of $\rho_1(0)$ for all fifty-five configurations has been used to obtain each $\rho(0)$. The process preserves the accuracy of the differences in density between configurations, which is our main concern.

TABLE II. Electron densities for various outer-electron configurations of iridium

N	$\rho_1(0)$	$\rho_2(0)$	$\rho_3(0)$	$\rho_4(0)$	$\rho_5(0)$	Total $\rho(0)$
<u>Iridium 5d^N configurations</u>						
0	3 599 847.8	398 088.8	88 979.3	21 659.8	4 221.1	4 112 796.7
1	398 080.2	88 968.5	21 649.0	4 123.3	4 112 668.8	
2	398 070.7	88 959.1	21 640.0	4 031.3	4 112 549.0	
3	398 067.0	88 951.0	21 632.5	3 945.9	4 112 444.2	
4	398 061.5	88 944.5	21 626.7	3 867.9	4 112 348.4	
5	398 057.9	88 939.3	21 622.4	3 798.4	4 112 265.8	
6	398 055.2	88 935.8	21 619.3	3 738.4	4 112 196.5	
7	398 052.9	88 933.1	21 617.4	3 689.8	4 112 141.0	
8	398 054.0	88 932.1	21 616.3	3 654.1	4 112 104.2	
9	398 054.0	88 931.7	21 616.0	3 632.2	4 112 081.7	

TABLE II. (Continued)

N	$\rho_1(0)$	$\rho_2(0)$	$\rho_3(0)$	$\rho_4(0)$	$\rho_5(0)$	$\rho_6(0)$	Total $\rho(0)$
<u>Iridium $5d^N 6s$ configurations</u>							
0	3 599 847.8	398 090.0	88 983.6	21 665.1	4 211.7	558.0	4 113 356.2
1		398 081.6	88 972.7	21 654.7	4 116.6	502.4	4 113 175.9
2		398 072.2	88 962.7	21 645.1	4 027.6	446.8	4 113 002.2
3		398 068.1	88 955.0	21 638.1	3 945.1	391.2	4 112 845.2
4		398 062.5	88 948.2	21 632.0	3 870.1	335.4	4 112 696.0
5		398 059.7	88 942.3	21 626.8	3 803.6	279.0	4 112 559.1
6		398 056.8	88 938.7	21 623.1	3 746.4	222.0	4 112 434.8
7		398 055.2	88 935.2	21 620.3	3 699.8	163.5	4 112 321.8
8		398 054.7	88 933.2	21 618.5	3 664.5	100.9	4 112 224.0
<u>Iridium $5d^N 6s^2$ configurations</u>							
0	3 599 847.8	398 090.4	88 986.6	21 671.7	4 221.6	1029.9	4 113 847.9
1		398 082.0	88 975.4	21 660.4	4 127.1	921.6	4 113 614.3
2		398 074.6	88 965.9	21 651.1	4 038.6	813.3	4 113 391.2
3		398 068.4	88 957.4	21 642.7	3 956.7	704.7	4 113 177.7
4		398 063.3	88 951.0	21 635.5	3 882.1	595.5	4 112 975.2
5		398 060.5	88 944.9	21 631.0	3 814.7	485.2	4 112 784.1
6		398 058.4	88 940.7	21 626.3	3 758.2	372.5	4 112 604.0
7		398 055.6	88 936.7	21 622.6	3 709.8	255.1	4 112 427.6
<u>Iridium $5d^N 6s6p$ configurations</u>							
0	3 599 847.8	398 086.6	88 981.6	21 662.0	4 196.1	525.7	4 113 299.8
1		398 077.0	88 970.4	21 652.0	4 103.8	470.8	4 113 121.7
2		398 070.4	88 961.1	21 643.1	4 017.6	416.0	4 112 955.9
3		398 066.5	88 953.6	21 636.2	3 938.0	361.2	4 112 803.2
4		398 060.6	88 946.7	21 630.5	3 865.8	306.3	4 112 657.7
5		398 058.1	88 942.3	21 626.2	3 801.7	251.3	4 112 527.3
6		398 056.5	88 938.5	21 622.7	3 746.6	196.1	4 112 408.1
7		398 054.7	88 935.3	21 620.4	3 700.6	141.2	4 112 299.9
<u>Iridium $5d^N 6s^2 6p$ configurations</u>							
0	3 599 847.8	398 087.5	88 984.6	21 668.2	4 206.5	968.1	4 113 762.7
1		398 077.2	88 972.8	21 657.7	4 114.7	861.4	4 113 531.5
2		398 071.6	88 964.4	21 648.7	4 028.9	754.7	4 113 316.1
3		398 067.5	88 956.5	21 641.2	3 949.6	648.1	4 113 110.8
4		398 062.5	88 949.9	21 634.9	3 877.5	541.1	4 112 913.7
5		398 058.7	88 944.6	21 629.5	3 813.3	433.8	4 112 727.7
6		398 057.5	88 940.4	21 625.6	3 757.0	326.4	4 112 554.7
<u>Iridium $5d^N 6s6p^2$ configurations</u>							
0	3 599 847.8	398 080.7	88 978.3	21 659.1	4 182.7	494.5	4 113 247.2
1		398 073.6	88 968.7	21 649.6	4 093.1	440.4	4 113 074.2
2		398 067.0	88 959.9	21 641.3	4 009.6	386.5	4 112 912.1
3		398 063.2	88 952.3	21 635.1	3 932.6	332.9	4 112 763.9
4		398 059.1	88 946.5	21 629.4	3 862.8	279.4	4 112 625.0
5		398 057.4	88 942.2	21 625.7	3 800.7	226.3	4 112 500.1
6		398 057.3	88 937.7	21 622.7	3 746.7	174.6	4 112 385.8
<u>Iridium $5d^N 6s^2 6p^2$ configurations</u>							
0	3 599 847.8	398 082.3	88 981.7	21 665.1	4 193.5	908.7	4 113 679.2
1		398 075.0	88 971.4	21 655.1	4 104.4	803.8	4 113 457.4
2		398 069.8	88 963.4	21 646.9	4 021.0	699.1	4 113 248.1
3		398 064.8	88 954.5	21 639.7	3 944.3	594.9	4 113 046.0
4		398 061.1	88 949.1	21 633.7	3 847.3	491.4	4 112 857.5
5		398 058.8	88 943.8	21 628.8	3 811.7	389.5	4 112 680.3

V. ANALYTICAL FIT TO DENSITY CALCULATIONS

To summarize the density results with a minimum of parameters, they were fitted to a simple analytical expression taking into account only lowest order shielding effects. If one considers a general configuration $5d^N 6s^M 6p^K$, the expression is

$$\rho(N, M, K) = \rho_{\text{inner}} + AM - \gamma_{ds} NM - \gamma_{ss} M(M - 1) - \gamma_{ps} KM. \quad (6)$$

In this expression, the first term ρ_{inner} is almost entirely dependent on N and only slightly on M and K. It contains the contributions of all inner shells ($n \leq 5$). We return to the M and K dependence of ρ_{inner} below. The term AM is the direct contribution of 6s electrons. However, it overemphasizes their effect because each electron added to 5d, 6s, and 6p somewhat shields the 6s electrons; the remaining three terms account for this shielding.

The term $\gamma_{ds} NM$ is the effect on the 6s central density due to the shielding of 5d electrons. The shielding is proportional to the number of electrons of each type and hence to the product NM. The term $\gamma_{ss} M(M - 1)$ is the effect of the shielding of 6s electrons upon each other. In the form given, it takes account of the impossibility of a 6s electron shielding itself. Finally, $\gamma_{ps} KM$ is the effect on the 6s central density due to the shielding of 6p electrons. Again the shielding is proportional to the number of electrons of each type and hence to the product KM. The quantities N, M, and K as used in Eq. (6) are necessarily integral. However, in a molecular orbital description of an iridium compound one must deal with nonintegral values. The form of the shielding terms in Eq. (6) is then to be modified, but the values of the constants are the same.

The term ρ_{inner} can be divided into three parts, a large contribution dependent on N alone, which we can write $\rho(N, 0, 0)$, and two small ones $\Delta\rho_s$ and $\Delta\rho_p$ which express the dependence of the central

density of inner shells on the population of 6s and 6p, respectively.

$$\rho_{\text{inner}} = \rho(N, 0, 0) + \Delta\rho_s(N, M, 0) + \Delta\rho_p(N, 0, K) \quad (7)$$

Inspection of Table II shows that the form of $\Delta\rho_s$ is such that it can be absorbed into the term AM. That is, we can write $A = A_{6s} + A_{\text{inner}}$, where A_{inner} is found to be about 2% of A. For our purpose it is not necessary to emphasize the distinction between the two contributions so only the value A need be used. The term $\Delta\rho_p(N, 0, K)$ is not negligible and can be fitted with an expression of the form

$$\Delta\rho_p(N, 0, K) = K(\eta - \zeta N), \quad (8)$$

with $\eta \approx 20$ and $\zeta \approx 4$. If the term is omitted, i.e., if in Eq. (6) we replace ρ_{inner} by $\rho(N, 0, 0)$ then an apparent N dependence of γ_{ps} arises so that it includes not only the shielding of 6p on the 6s central density but also minor effects upon inner shells. It is not particularly less convenient to let γ_{ps} vary with N, but for many purposes it is sufficient to use the simple approximation $\gamma_{ps} = \gamma_{ss}$, which is correct at $N \approx 2.5$.

It is convenient to have $\rho(N, 0, 0)$ in analytic form also, although we offer no theoretical justification for the form found. A good fit can be obtained by writing

$$\rho(N, 0, 0) = a + \gamma_{di}(10 - N)^2, \quad (9)$$

a parabola centered at $N = 10$, the value for the filled d shell. The shielding constant γ_{di} in the expression is the shielding of the central density of inner shells by 5d electrons.

Figure 3 shows the Hartree-Fock densities along with the densities obtained from a least-squares fit to Eq. (6). The abscissae are the ionization state $9 - (M + N + K)$. The values for A, γ_{ds} , and γ_{ss} are obtained from fitting the differences $\rho(N, M, 0) - \rho_{\text{inner}}$,

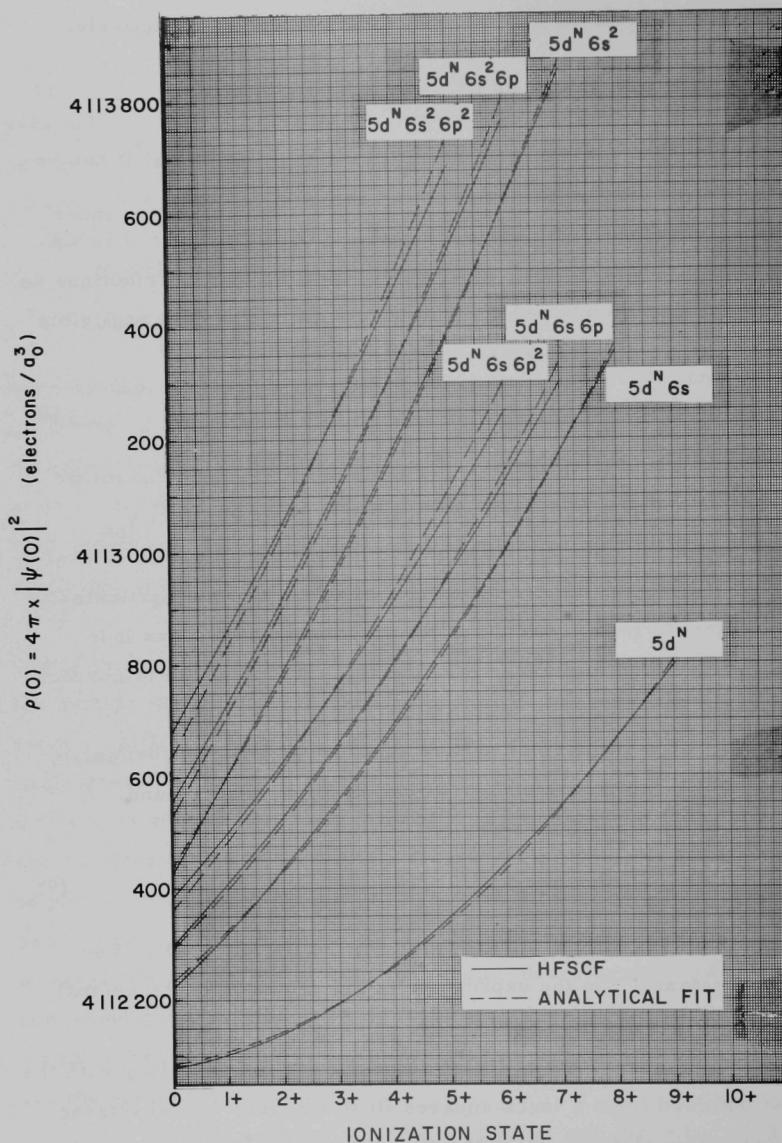


Fig. 3. HFSCF electron-density calculations and the analytical fit to Eq. (6).

where we have assumed that $\rho_{\text{inner}} = \rho(N, 0, 0)$ and that γ_{ps} varies with N. The N dependence of γ_{ps} is such that $\gamma_{\text{ps}} \approx 0.8\gamma_{\text{ss}}$ for the neutral atom and $\gamma_{\text{ps}} \approx 1.7\gamma_{\text{ss}}$ for highly ionized cases. The parameter values used in plotting Fig. 3 were

$$\begin{aligned} a &= 4 \ 112 \ 075.8, & \gamma_{\text{di}} &= 7.27, & A &= 562 \\ \gamma_{\text{ds}} &= 54.4, & \gamma_{\text{ss}} &= 33.7, & \gamma_{\text{ps}} &= \gamma_{\text{ss}}. \end{aligned} \quad (10)$$

Figure 3 shows that the fit is excellent except for configurations containing 6p electrons. The deviations in the $5d^N 6s$ and $5d^N 6s^2$ curves are almost entirely due to the deviations in the fit to Eq. (9). The poorer but still respectable fit to configurations with 6p electrons arises in large part from the N dependence in ρ_{inner} .

We may also restate Eq. (6) in an alternative form that gives more insight into the magnitude of the shielding constants by referring the density to that of an arbitrary configuration. For the latter we choose $\text{Ir}^- (5d^{10})$. Then

$$\begin{aligned} \delta \rho &\equiv \rho(N, M, K) - \rho(10, 0, 0) \\ &= A [M + \gamma'_{\text{di}} (10 - N)^2 - \gamma'_{\text{ds}} NM - \gamma'_{\text{ss}} M(M - 1) - \gamma'_{\text{ps}} KM], \end{aligned} \quad (6')$$

where the values of the primed parameters are

$$\begin{aligned} A &= 562, & \gamma'_{\text{di}} &= 0.0129, & \gamma'_{\text{ss}} &= 0.060, \\ \gamma'_{\text{ds}} &= 0.097, & \gamma'_{\text{ps}} &= \gamma'_{\text{ss}}. \end{aligned} \quad (11)$$

The addition of one 5d electron is observed to reduce the contribution of a 6s electron by the amount $\gamma'_{\text{ds}} = 0.097$ electron. Similarly, the addition of the second 6s electron reduces the contribution of the first one by $\gamma'_{\text{ss}} = 0.060$ electron and the latter shields the former by the same amount. The addition of an electron to 6p acts as if it reduces the density of a 6s electron by a variable amount γ'_{ps} depending on N, with $\gamma'_{\text{ps}} = \gamma'_{\text{ss}}$ at $N \approx 2.5$.

ACKNOWLEDGMENTS

The authors are indebted to M. Wilson and M. Fred for insight into the operation of the computer program and to J. Oyler for some of the calculations. We also wish to thank F. Throw for editorial assistance.

ARGONNE NATIONAL LAB WEST



3 4444 00008237 0

X

